

IN THE CLAIMS:

Amend the claims as follows:

Claims 1-4. (Canceled)

5. (Currently Amended) A method for identifying an agent compound which modulates ketopantoate hydroxymethyltransferase (KPHMT) activity, comprising the steps of:

- (a) employing three-dimensional atomic coordinate data according to Table 1 to characterise at least one KPHMT binding ~~sites~~ sites;
- (b) providing the structure of a candidate agent compound;
- (c) fitting the candidate agent compound to the binding sites; and
- (d) selecting the candidate agent compound.

6. (Original) The method of claim 5 wherein:
a plurality of binding sites are characterised and a plurality of agent compounds are fitted to said sites; and
said agent compounds are linked to form a potential modulator compound.

7. (Original) The method of claim 5 wherein step (b) comprises selecting said candidate agent compound by computationally screening a database of compounds for interaction with said binding site.

8. (Original) The method of claim 5 which comprises the further steps of:
(e) obtaining or synthesising the candidate agent compound; and
(f) contacting the candidate agent compound with KPHMT to determine the ability of the candidate agent compound to interact with KPHMT.

Claims 9-10. (Canceled)

11. (Currently Amended) A method for determining the structure of a KPHMT homologue of the ketopantoate hydroxymethyltransferase (KPHMT) defined by Table 1, wherein said method comprises:

(a) aligning a representation of an amino acid sequence of a KPHMT homologue of unknown structure with the amino acid sequence of KPHMT to match homologous regions of the amino acid sequences;

(b) modelling the structure of the matched homologous regions of the KPHMT of unknown structure on the structure as defined by Table 1 of the corresponding regions of the KPHMT of Table 1; and

(c) determining a conformation for the KPHMT of unknown structure which substantially preserves the structure of said matched homologous regions.

Claims 12-13. (Canceled)

14. (new) A computer-based method of rational drug design which comprises:
providing the structure of the ketopantoate hydroxymethyltransferase (KPHMT) as defined by the coordinates of Table 1 or a root mean square deviation from the backbone atoms of less than 1.5 Å thereof;

providing the structure of a candidate agent compound; and

fitting the structure of the candidate to said structure of the KPHMT as defined by the coordinates of Table 1 or a root mean square deviation from the backbone atoms of less than 1.5 Å thereof.

15. (new) The method of claim 5 wherein said at least one KPHMT binding site is characterised by employing atomic coordinate data for at least two atoms from the

atoms of the residues Tyr25, Asp45, Ser46, Asp84, Lys112, Glu114, Tyr150, Lys151, Arg155, Glu181, Asp217, Lys228, Lys231, Phe229 and His261.

16. (new) The method of claim 5 wherein said atomic coordinate data includes data for KPHMT backbone atoms, the positions of said backbone atoms varying by less than a root mean square deviation of 1.5 Å from the corresponding positions of Table 1.